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The Korteweg Theory of Cappilarity and the Phase Transition Problems *

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Abstract

In this paper we first summarize the earlier results on the slow motion in the Korteweg theory of cappilarity in the one-dimensional case and show some numerical results. In the multidimensional case we discuss the existence of local solutions to the system of equations for compressible fluids of Korteweg type.

1 Introduction

In order to model the capillarity effect of materials, Korteweg [12] formulated a constitutive equation for the Cauchy stress that includes density gradients. It turns out that his theory is useful to discuss phase transition problems.

First, we discuss the one-dimensional isothermal motion. In this case the equation we discuss is given by

$$u_{tt} = \sigma(u_x)_x + \nu u_{xxt} - \epsilon^2 u_{xxxx}, \quad 0 < x < 1, \quad t > 0. \tag{1.1}$$

where u is the displacement and u_{xxt} and u_{xxxx} terms represent the viscosity and the capillarity effects, respectively. Typical boundary conditions come from either a soft loading device or a hard loading device. Although the slow motion occurs in both cases, in this note we discuss the soft loading case only for simplicity. The boundary conditions in this case are given by

$$\begin{gathered} u(0,t) = 0, \quad \sigma(u_x) + \nu u_{xt} - \epsilon^2 u_{xxx}|_{x=1} = P, \\ u_{xx}(0,t) = 0, \quad u_{xx}(1,t) = 0. \end{gathered} \tag{1.2}$$

The initial conditions are given by

$$u(x,0) = f(x), \quad u_t(x,0) = g(x), \tag{1.3}$$

where $f, g \in H^1(0,1)$. The boundary conditions (1.2a) show that the stress P is applied at $x = 1$. The boundary conditions (1.2b) are the natural boundary conditions for the corresponding variational problem.

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In what follows, we assume that σ is given by Fig. 1.1. In this figure $(0, \alpha^*]$ and $[\beta^*, \infty)$ are called the α-phase and the β-phase, respectively. They correspond to the different phases of the material. The interval (α^*, β^*) is called the spinodal region and physically unstable. We denote by α, δ, and β the values of u_x at the intersections of $y = P$ and $y = \sigma(u_x)$ in the α-phase, the spinodal region, and the β-phase, respectively. The value of P for which areas A and B are equal is called the Maxwell line. We denote by α_M, β_M, and δ_M the values of α, β, and δ, respectively, for which we have the Maxwell line construction.

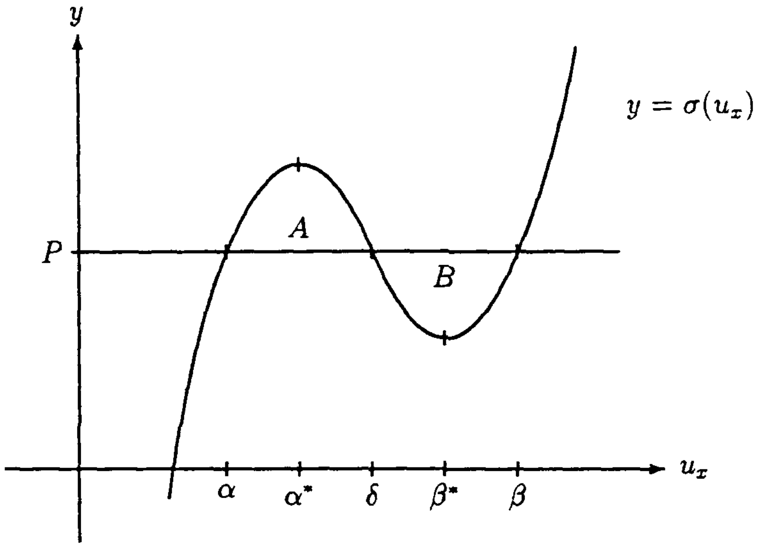


Figure 1.1

The capillarity term was first introduced by Korteweg [12]. Recently, various effects of this term have been discussed. For example, Serrin [15], [16] reconsidered the Korteweg theory and has shown the existence of steady profile connecting the α-phase and the β-phase. Slemrod [17] and Hagan and Slemrod [9] considered the existence of travelling wave solutions. The static problems concerning the soft loading case and the hard loading case have been discussed in [3] and [4], respectively. The dynamical aspects of these loading cases are discussed in Hattori and Mischaikow [10] and Andrews and Ball [1].

In Section 2 we summarize the result in [11] about a slow motion of (1.1) resembling the dynamics of (2.3) discussed in [7], [5], [2], and [8]. In Section 3 we show some numerical examples of slow motions. In Section 4 we dsicuss the existence of local solutions to the system of equations for two dimensional isothermal motion of compressible fluids of Korteweg type. The higher order terms of density (or the deformation gradient) in the Cauchy stress tensor is not in general compatible with the classical theory of thermodynamics. Dunn and Serrin [6] introduced the concept of interstitial working and derived the Cauchy stress tensor compatible with thethermodynamics. First, we summarize their results and derive the system of equations. Then, we state the theorem for the existence of local solutions.

2 Slow motions one-dimensional case

In this section we summerize the results in [2], [8], and [11]. Multiply (1.1) by u_t, integrate in x and t, and then integrate by parts using (1.2). After dividing by ϵ, we have,

$$E[u](t) + \frac{1}{\epsilon}\int_0^t \int_0^1 \nu u_{xt}^2(x,s)\,dxds = E[u](0), \tag{2.1}$$

where

$$E[u](t) = \int_0^1 \{\frac{1}{2\epsilon}u_t^2 + \frac{1}{\epsilon}(W(u_x) - Pu_x) + \frac{\epsilon}{2}u_{xx}^2\}(x,t)\,dx. \tag{2.2}$$

In (2.2) $W(u_x)$ is a primitive of σ. For the remainder of the paper we shall assume that $P = \sigma(\alpha_M)$. This implies that $W(u_x) - Pu_x$ will be double-well potentials with equal depth. For the sake of simplicity we shall also assume that $W(u_x) - Pu_x$ is given by $(u_x - 1)^2$. The same conclusions will hold for more general non-linearities.

Observe that (2.1) is similar to that for the parabolic equation

$$\nu v_t = \epsilon^2 v_{xx} - (v^3 - v), \tag{2.3}$$

with either the homogeneous Neumann boundary condition

$$v_x(0,t) = 0, \quad v_x(1,t) = 0$$

or a Dirichlet condition

$$v(0,t) = a, \quad v(1,t) = b, \quad a, b = \pm 1.$$

In particular the energy relation for (2.3) is given by

$$E_p[v](t) + \frac{1}{\epsilon}\int_0^t \int_0^1 \nu v_t^2(x,s)\,dxds = E_p[v](0), \tag{2.4}$$

where

$$E_p[v](t) = \int_0^1 \{\frac{1}{4\epsilon}(v^2 - 1)^2 + \frac{\epsilon}{2}v_x^2\}(x,t)\,dx. \tag{2.5}$$

Now we summarize the results of the slow motions for the parabolic equation. We assume for the initial data of (2.3) that

$$w(x) = \lim_{\epsilon \to 0} v^\epsilon(x,0) \tag{2.6}$$

exists as a limit of L^1 norm, where w is a piecewise constant function taking only the values ± 1, with exactly N discontinuities at $\{x_1, \cdots, x_N\}$ and we also assume that the initial data satisfy

$$E_p[v^\epsilon](0) \leq Nc_o + K_2 \exp(-K/\epsilon). \tag{2.7}$$

Then, we have

Lemma 2.1 *Suppose the initial data for (2.3) satisfy (2.6) and (2.7). Then, for any T satisfying $0 \leq T \leq F\nu\epsilon^s \exp(-K/\epsilon)$, we have*

$$\sup_{0 \leq t \leq T} \int_0^1 |v^\epsilon(x,t) - v^\epsilon(x,0)|\, dx \leq (FG)^{1/2} \epsilon^{\frac{1}{2}(s+1)}. \tag{2.8}$$

Next, we summarize the results concerning the slow motions of (1.1). As the form of the energy relation (2.1) resembles (2.4), we can expect to draw the same kind of conclusions for (1.1). For this purpose we rewrite the energy $E_c[u]$ as

$$E_c[u] = E_s[u] + E_p[u_x], \quad E_s[u] = \int_0^1 \frac{1}{2\epsilon} u_t^2(x,t)\, dx.$$

We assume that the initial data for (1.1) satisfy

$$u_x^\epsilon(x,0) = v^\epsilon(x,0) \tag{2.9}$$

and

$$E_s[u^\epsilon](0) \leq C \exp(-K/\epsilon). \tag{2.10}$$

The condition (2.9) is imposed for the sake of simplicity. As long as $u_x(x,0)$ satisfies (2.6) and (2.7), with v being replaced by u_x, the same conclusion should be obtained.

Lemma 2.2 *Suppose (2.9) and (2.10) are satisfied. Then, for any T satisfying $0 \leq T \leq F_c\nu\epsilon^s \exp(K/\epsilon)$, the solution to (1.1) satisfies*

$$\sup_{0 \leq t \leq T} \int_0^1 |u_x^\epsilon(x,t) - u_x^\epsilon(x,0)|\, dx \leq (F_cG_c)^{1/2} \epsilon^{\frac{1}{2}(s+1)}. \tag{2.11}$$

Using Nirenberg's inequality and Lemmas 2.1 and 2.2, we can show

Theorem 2.3 *If $s > 1$, then the difference in the L^∞ norm between u_x^ϵ and v^ϵ is $O(\epsilon^{\frac{1}{6}(s-1)})$ for at least $0 \leq t \leq F_m\nu\epsilon^s \exp(K/\epsilon)$, where $F_m = \min\{F, F_c\}$.*

3 Numerical examples

We give a numerical exmaple of the soft loading case to confirm the results in the previous section. We introduce the transform

$$p = \int_1^x u_t(x,t)\,dx, \quad q = u_x$$

similar to Pego's [14]. Then, (1.1) becomes

$$\begin{aligned} p_t &= \nu p_{xx} - \eta q_{xx} + \sigma(q) - P, \\ q_t &= p_{xx}. \end{aligned} \tag{3.1}$$

The boundary conditions for p and q become

$$\begin{aligned} p_x(0,t) = 0, \quad p(0,t) = 0, \\ q_x(0,t) = 0, \quad q_x(1,t) = 0. \end{aligned} \tag{3.2}$$

For the initial condition, we consider the case when

$$p(x,0) = 0, \quad q(x,0) = Cf(x), \tag{3.3}$$

where C is a parameter representing the magnitude of initial data.

As an example, we consider the case when $\epsilon = 0.01$, $\nu = 1.0$, and the initial data for the parabolic equation and for (3.1) are given, respectively, by

$$v(x,0) = C(\cos 2\pi x + \cos 9\pi x),$$

$$p(x,0) = 0, \quad q(x,0) = v(x,0).$$

For C we gave the following values:

$$C = 1.0, 0.5, 0.1, 0.01, 0.001.$$

One of the reasons why we change the magnitude of the initial data is to see how this influences the metastable states. We should note that for either choice of C above, the conditions (2.9) and (2.10) are not satisfied. Nevertheless, when $C = 1.0, 0.5, 0.1$, v and q have reached the same metastable state in each case. Here, we show the numerical results of $C = 0.1, 0.01$ only. In Figures 3.1 and 3.2 we show how v and q evolve for $0 \le t \le 10$ and then in Figures 3.3 and 3.4 we show the profiles of v and q at $t = 1000$. We use the solid lines for v and the gray lines for q. When these lines overlap, we see only the gray lines. When $C = 0.1$, they agree at least to 10^{-7} at $t = 1000$ and this agreement continues at least until $t = 10000$. In these figures, the values of x should be multiplied by 0.01.

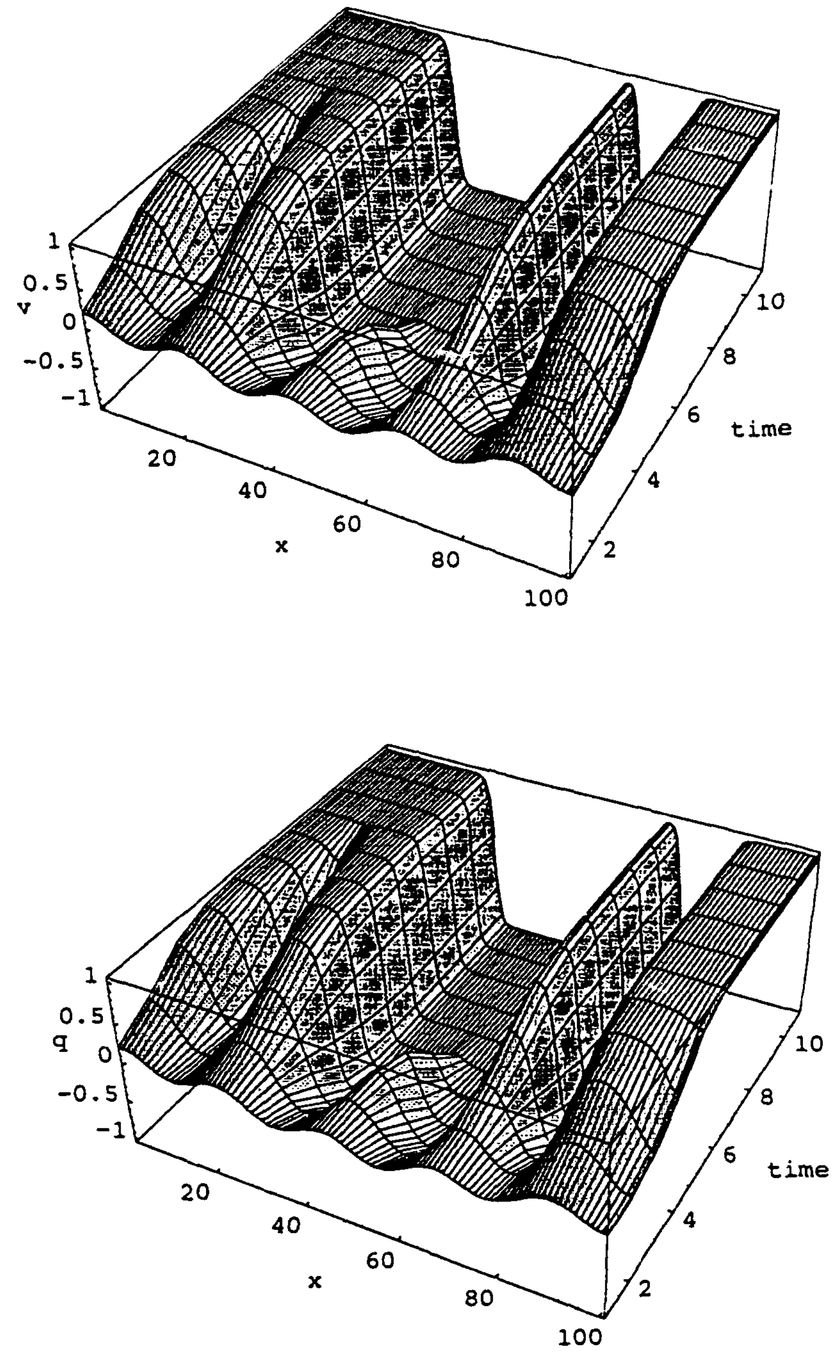
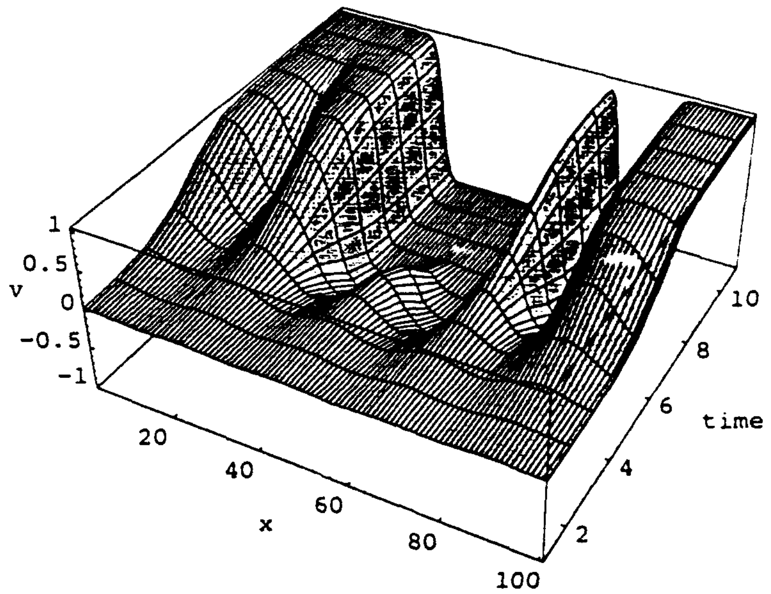


Figure 3.1. v and q for $C = 0.1$, $0 \leq t \leq 10$.



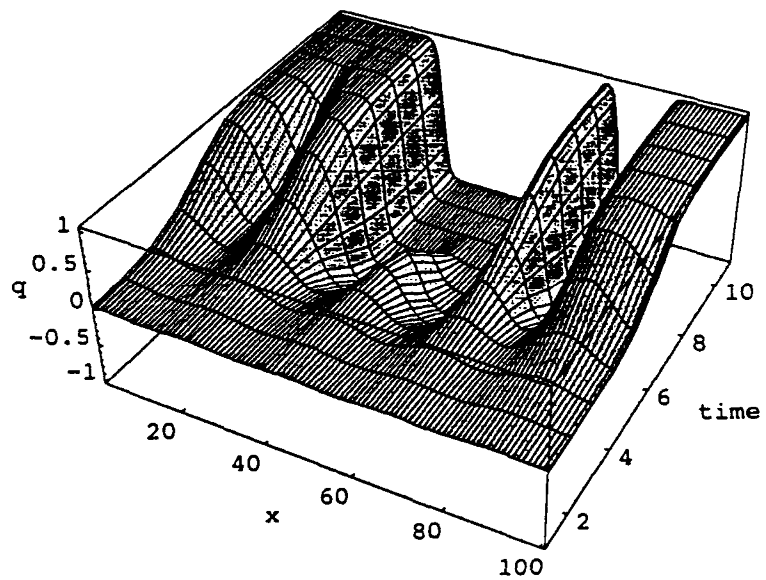


Figure 3.2. v and q for $C = 0.01$, $0 \leq t \leq 10$.

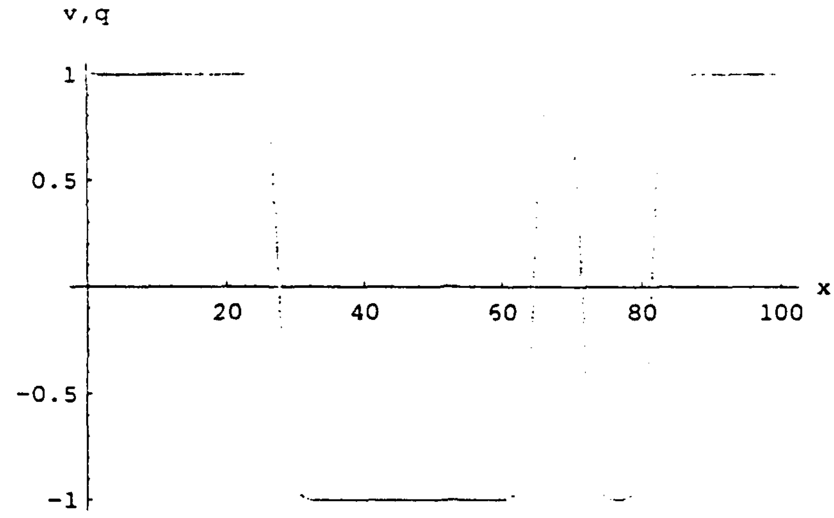


Figure 3.3. v and q at $t = 1000$ for $C = 0.1$.

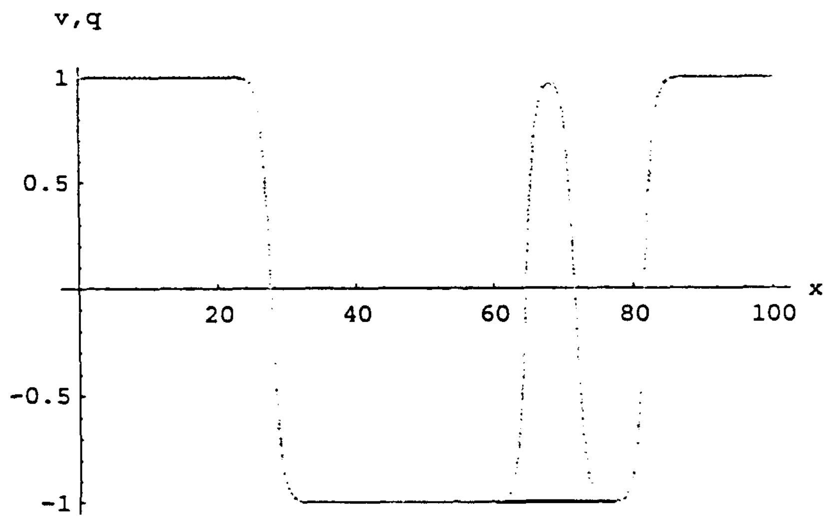


Figure 3.4. v and q at $t = 1000$ for $C = 0.01$.

4 Local existence in multidimensional case

Dunn and Serrin [6] modified the Korteweg theory and derived the following set of equations for the conservation of mass, the balance of linear momentum, the balance of energy, and the Clausius-Duhem inequality:

$$
\begin{aligned}
&\rho_t + \mathrm{div}(\rho\mathbf{u}) = 0, \\
&\rho\frac{D\mathbf{u}}{Dt} = \mathrm{div}\mathbf{T}, \\
&\rho\frac{D\varepsilon}{Dt} = \mathbf{T}\cdot\mathbf{L} - \mathrm{div}\mathbf{q} + \mathrm{div}\mathbf{w}, \\
&\rho\theta\frac{D\eta}{Dt} + \mathrm{div}\mathbf{q} + \frac{\mathbf{q}\cdot(\mathrm{grad}\theta)}{\theta} \geq 0,
\end{aligned} \tag{4.1}
$$

where $\frac{Df}{Dt} = f_t + \mathbf{u}\cdot\nabla f$ and

1. $\rho = \rho(\mathbf{x}, t)$ is the density of the fluid at the point $\mathbf{x}$ at time t,
2. $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ is the velocity of fluid,
3. $\theta = \theta(\mathbf{x}, t)(> 0)$ is the absolute temperature,
4. $\varepsilon = \varepsilon(\mathbf{x}, t)$ is the specific internal energy per unit mass,
5. $\eta = \eta(\mathbf{x}, t)$ is the specific entropy per unit mass,
6. $\mathbf{T} = \mathbf{T}(\mathbf{x}, t)$ is the Cauchy stress tensor,
7. $\mathbf{q} = \mathbf{q}(\mathbf{x}, t)$ is the heat flux vector,
8. $\mathbf{L} = \mathrm{grad}\mathbf{u}$.

The main difference with the classical thermodynamics is the $\mathrm{div}\mathbf{w}$ term and $\mathbf{w}$ is called the interstitial work flux representing spacial interactions of longer range. They have proved that for a given Helmholtz free energy $\psi(\rho, \theta, \mathbf{d})$, the following forms of $\mathbf{w}$ and $\mathbf{T}$

$$
\begin{aligned}
\mathbf{w} &= \rho\dot{\rho}\psi_{\mathbf{d}} + \bar{\mathbf{w}}, \\
\mathbf{T} &= (-\rho^2\psi_\rho + \rho\mathbf{d}\cdot\psi_{\mathbf{d}} + \rho^2\nabla\cdot\psi_{\mathbf{d}})\mathbf{I} - \rho\mathbf{d}\otimes\psi_{\mathbf{d}}
\end{aligned} \tag{4.2}
$$

are compatible with (4.1d). Here, $\rho^2\psi_\rho(\rho, \theta, 0)$ is the pressure and $\bar{\mathbf{w}}$ is the "static" portion of the interstitial work flux $\mathbf{w}$. They have shown that if the material possesses a center of symmetry, $\bar{\mathbf{w}} = 0$. In what follows, we consider the materials which posess the center of symmetry. They also have observed that the classical forms of viscosity and conductivity tensors are compatible.

In this note we state a result concerning the existence of a unique local smooth solution in the two-dimensional isothermal motion of the Korteweg type materials where the viscous effect is also included. The 3-dimensional case can be discussed similarly. In what follows, we state the assumptions on the Helmholtz free energy and derive the system that we shall discuss. We assume that the Helmholtz free energy is given by

$$\psi = F(\rho) + \frac{\nu}{2\rho}(\rho_x^2 + \rho_y^2), \tag{4.3}$$

where F is a smooth function of ρ and ν is a positive constant. This choice is to make the terms appearing in (4.4) as simple as possible, yet to reflect the effect of the higher order terms of ρ. [1]

With the choice the Helmholtz free energy given in (4.3) and with $\lambda = -\frac{1}{3}\mu$, the system then becomes

$$\begin{aligned} &\rho_t + (\rho u)_x + (\rho v)_y = 0, \\ &(\rho u)_t + (\rho u^2)_x + (\rho uv)_y = (T_{11})_x + (T_{12})_y, \\ &(\rho v)_t + (\rho uv)_x + (\rho v^2)_y = (T_{21})_x + (T_{22})_y, \end{aligned} \tag{4.4}$$

where u and v are the x and y component of velocity and

$$\begin{aligned} \mathbf{T} &= \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \\ &= \left\{-p + \frac{\nu}{2}(\rho_x^2 + \rho_y^2) + \nu\rho\Delta\rho\right\}\mathbf{I} - \nu \begin{pmatrix} \rho_x^2 & \rho_x\rho_y \\ \rho_x\rho_y & \rho_y^2 \end{pmatrix} + \mathbf{V}, \end{aligned} \tag{4.5}$$

$$p = \rho^2 F'(\rho), \tag{4.6}$$

and

$$\begin{aligned} \mathbf{V} &= \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} \\ &= \mu\{(\text{gradu}) + (\text{gradu})^T - \frac{2}{3}(\text{divu})\mathbf{I}\}. \end{aligned} \tag{4.7}$$

Here, $\mathbf{I}$ is the unit rank-two tensor and a superscript T denotes the transpose of a tensor. Since we discuss the existence of a local solution, we do not need the monotonicity of the pressure on ρ. Further computation simplifies the div$\mathbf{T}$ term

$$\text{div}\mathbf{T} = -\nabla p + \nu\rho\nabla(\Delta\rho) + \text{div}\mathbf{V}. \tag{4.8}$$

We discuss the local existence for the pure initial value problem of (4.4) with the initial data given by

$$(\rho, u, v)(x, y, 0) = (\rho_o, u_o, v_o)(x, y). \tag{4.9}$$

[1] Another reasonable choice is to change the last term in (4.3) with $\frac{\nu}{2}(\rho_x^2 + \rho_y^2)$. Although this choice may be physically more realistic, mathematically it is more cumbersome to handle. For example, the expression for div$\mathbf{T}$ is very complicated. Therefore, we do not discuss this case (See (4.8)).

We assume that the initial data satisfy

$$(\rho_0 - \bar{\rho}_0, u_0, v_0) \in H^k(R^2), \qquad \bar{\rho}_o \geq \delta > 0, \tag{4.10}$$

where $k \geq 4$ and $\bar{\rho}_0 > 0$ is a positive constant. Denote by $\|\cdot\| \equiv \|\cdot\|_o$ the L^2 norm and by $\|\cdot\|_k$ the k-th order Sobolev norm. Set

$$\|w\|_{0,T}^2 \equiv \sup_{0\leq t\leq T} \left(\|w(t)\|^2 + \|\nabla\rho(t)\|^2\right) + \int_0^T \left(\|\nabla u(t)\|^2 + \|\nabla v(t)\|^2\right) dt$$

and

$$\|w\|_k^2 = \sum_{|j|\leq k} \|\partial_{x,y}^j w\|^2,$$

where $w \equiv (\rho, u, v)$. The main result is stated as follows.

Theorem 4.1 *For any initial data (ρ_0, u_0, v_0) such that $\rho_0 \geq \delta > 0$ and $(\rho_0 - \bar{\rho}_0, u_0, v_0) \in H^k(R^2)$ $(k \geq 4)$ where $\bar{\rho}_0 > 0$ is a constant, there exists a $T > 0$ such that in $t \in [0, T]$, the Cauchy problem (4.4), (4.9) has a unique solution (ρ, u, v) such that $\rho - \bar{\rho}_0 \in L^\infty([0,T]; H^{k+1}(R^2))$ and $(u, v) \in L^\infty([0,T]; H^k(R^2))$ and*

$$\|w\|_k^2 \leq C_k\|w_0\|_k^2 + \|\rho_0\|_{k+1}^2.$$

Since the linearized problem of (4.4), (4.9) is not of any classical type, the existence of solutions is not known even for the linearzed problem. We prove the existence of solutions for the linearized problem by establishing an energy estimate for the dual problem and then using the dual argument.

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